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Dependence of the Log K Values for the Interaction of Chiral Dimethylpyridino-18-crown-6 with α-(1-Naphthylethyl)ammonium Perchlorate on Several Solvent Parameters

12. PERSONAL AUTHOR(S)
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The log K values for the complexation of chiral dimethylpyridino-18-crown-6 with the (R)- and (S)- enantiomers of α-(1-naphthylethyl)ammonium perchlorate were determined by the direct ^1H NMR technique[1] in a variety of solvents. The crown and salt are shown in Figure 1 along with the log K values. It is clear from the data in Figure 1 that the magnitude of log K correlates well with the solvent donor number (DN) but there is no correlation between log K values and the dielectric constant (ε_r), acceptor number (AN) or empirical polarity (E_T^N) of each solvent. Solvents with low donor numbers allowed the most stable complexation as would be expected. Solvents with high donor numbers would form strong solvent associations with the guest so that guest molecules would be less available for the chiral ligand. DMSO-d_6 associates so strongly with the ammonium salt that no complexation with the ligand was observed.

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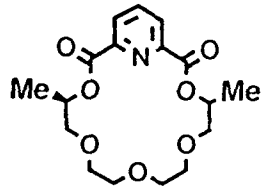
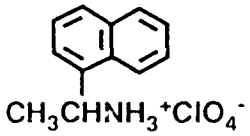
It is interesting that three of these systems exhibited the same recognition for the (S)-salt over the (R)-form as shown by the fact that the Δ log K values were about equal (0.42 to 0.44). More work needs to be done with these systems to understand these results.

(1) C.Y. Zhu, J.S. Bradshaw, J.L. Oscarson, and R.M. Izatt, "Evaluation of a Direct ^{1}H NMR Method for Determining log K and ΔH Values for Crown Ether–Alkylammonium Cation Complexation," J. Incl. Phenom., in press (also Technical Report No. 13 to ONR by the same authors, October 24, 1990).

Dependence of Log K on Several Solvent Parameters

For  + 

(R,R) (R) or (S)

Solvent	Solvent Parameters[a]				Log K[b]		ΔLog K
	ε_r	DN	AN	E_T^N	(R)	(S)	
CD_3NO_2	35.94	*2.7*	20.5	0.481	~5.50	-[c]	-
CD_3CN	35.94	*14.1*	12.5	0.460	3.80	4.24	0.44
CD_3COCD_3	20.56	*17.0*	12.5	0.355	2.98	3.40	0.42
CD_3OD	32.66	*19.0*	41.5	0.762	2.08	2.50	0.42
DMSO-d_6	46.45	*29.8*	19.3	0.444	NR[d]	NR	-

[a] ε_r = dielectric constant, DN = donor number, AN = acceptor number, and E_T^N = empirical polarity.

[b] Temperature is 25.0 °C.

[c] Log K is too big to measure by the NMR method.

[d] No reaction.